	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 08:32:43 ON 07 AUG 2007

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STRUCTURE FILE UPDATES: 6 AUG 2007 HIGHEST RN 944108-38-7
DICTIONARY FILE UPDATES: 6 AUG 2007 HIGHEST RN 944108-38-7

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http://www.cas.org/support/stngen/stndoc/properties.html

=> E "2-IMIDAZOLYL DISULFIDE"/CN 25
E1 1 2-IMIDAZOLONE-4,5-DICARBONITRILE/CN
E2 1 2-IMIDAZOLYL DIETHYLDITHIOCARBAMATE/CN
E3 0 --> 2-IMIDAZOLYL DISULFIDE/CN
E4 1 2-IMIDAZOLYL KETONE, PICRATE/CN
E5 1 2-IMIDAZOLYL METHYL KETONE/CN
E6 1 2-IMIDAZOLYL-1-(2-THIENYL)ETHANOL/CN
E7 1 2-IMIDAZOLYL-2'-ACETONAPHTHONE/CN
E8 1 2-IMIDAZOLYL-5-BROMOPYRIDINE/CN
E9 1 2-IMIDAZOLYL-5-FORMYLPYRIDINE/CN
E10 1 2-IMIDAZOLYL-5-HYDROXYMETHYLPYRIDINE/CN
E11 1 2-IMIDAZOLYLACETYLENE/CN
E12 1 2-IMIDAZOLYLFORMALDEHYDE/CN
E13 1 2-IMIDAZOLYLMETHYL-4-BROMOPYRIDINE/CN
E14 1 2-IMINIOPROPANE-1,3-DIYL CONJUGATE ACID/CN
E15 1 2-IMINO(1,2,4)OXADIAZOLO(2,3-A)QUINOLINE MONOHYDROBROMIDE/CN
E16 1 2-IMINO-A-PHENYL-3(2H)-THIAZOLEETHANOL/CN
E17 1 2-IMINO-1,2-DIHYDROCYCLOHEPTA(B)PYRROLE/CN
E18 1 2-IMINO-1,2-DIHYDROPYRIDINE-1-ACETIC ACID/CN
E19 1 2-IMINO-1,3-BENZOTHIAZIN-4-ONE/CN
E20 1 2-IMINO-1,3-DIAZACYCLOHEPTANE/CN
E21 1 2-IMINO-1,3-DITHIETANE HYDROCHLORIDE/CN
E22 1 2-IMINO-1,3-DITHIOLANE HYDROCHLORIDE/CN
E23 1 2-IMINO-1,3-DITHIOLANE-4-CARBOXYLIC ACID HYDROCHLORIDE/CN
E24 1 2-IMINO-1,3-THIAZANONE-4/CN
E25 1 2-IMINO-1,4-DIMETHYL-1,2-DIHYDROPYRIMIDINE/CN

=> E "2-MERCAPTOIMIDAZOLE"/CN 25
E1 1 2-MERCAPTOHYDROQUINONE/CN
E2 1 2-MERCAPTOHYPOXANTHINE/CN
E3 1 --> 2-MERCAPTOIMIDAZOLE/CN
E4 1 2-MERCAPTOIMIDAZOLE-4-ACRYLIC ACID/CN
E5 1 2-MERCAPTOIMIDAZOLIDINE/CN
E6 1 2-MERCAPTOIMIDAZOLINE/CN
E7 1 2-MERCAPTOIMIDAZOLINE, ZINC SALT/CN
E8 1 2-MERCAPTOINDOLE/CN
E9 1 2-MERCAPTOINOSINE PYRIDINIUM SALT/CN

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 NEWS  2  MAY 01  New CAS web site launched
 NEWS  3  MAY 08  CA/CAplus Indian patent publication number format defined
 NEWS  4  MAY 14  RDISCLOSURE on STN Easy enhanced with new search and display
                  fields
 NEWS  5  MAY 21  BIOSIS reloaded and enhanced with archival data
 NEWS  6  MAY 21  TOXCENTER enhanced with BIOSIS reload
 NEWS  7  MAY 21  CA/CAplus enhanced with additional kind codes for German
                  patents
 NEWS  8  MAY 22  CA/CAplus enhanced with IPC reclassification in Japanese
                  patents
 NEWS  9  JUN 27  CA/CAplus enhanced with pre-1967 CAS Registry Numbers
 NEWS 10  JUN 29  STN Viewer now available
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 NEWS 12  JUL 02  LEMBASE coverage updated
 NEWS 13  JUL 02  LMEDLINE coverage updated
 NEWS 14  JUL 02  SCISEARCH enhanced with complete author names
 NEWS 15  JUL 02  CHEMCATS accession numbers revised
 NEWS 16  JUL 02  CA/CAplus enhanced with utility model patents from China
 NEWS 17  JUL 16  CAplus enhanced with French and German abstracts
 NEWS 18  JUL 18  CA/CAplus patent coverage enhanced
 NEWS 19  JUL 26  USPATFULL/USPAT2 enhanced with IPC reclassification
 NEWS 20  JUL 30  USGENE now available on STN
 NEWS 21  AUG 06  CAS REGISTRY enhanced with new experimental property tags
 NEWS 22  AUG 06  BEILSTEIN updated with new compounds
 NEWS 23  AUG 06  FSTA enhanced with new thesaurus edition

 NEWS EXPRESS  29 JUNE 2007:  CURRENT WINDOWS VERSION IS V8.2,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

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FILE 'HOME' ENTERED AT 08:32:25 ON 07 AUG 2007

=> file reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
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```
E10             1      2-MERCAPTOISOBUTANOIC ACID/CN
E11             1      2-MERCAPTOISOBUTYRIC ACID/CN
E12             1      2-MERCAPTOISONICOTINIC ACID/CN
E13             1      2-MERCAPTOISOPHTHALIC ACID/CN
E14             1      2-MERCAPTOISOPROPYL ETHER/CN
E15             1      2-MERCAPTOISOPROPYLAMINE HYDROCHLORIDE/CN
E16             1      2-MERCAPTOLAURIC ACID/CN
E17             1      2-MERCAPTOLEPIDINE/CN
E18             1      2-MERCAPTOMESITYLENE/CN
E19             1
2-MERCAPTOMETHYL)-N,N'-BIS(2-MERCAPTO-2-METHYLPROPYL)-2-METHYLPROPANEDIAMIDE/CN
E20             1      2-MERCAPTOMETHYL-1,3-DITHIOLANE/CN
E21             1      2-MERCAPTOMETHYL-1,3-PROPANEDITHIOL-M-XYLYLENE DIISOCYANATE
COPOLYMER/CN
E22             1      2-MERCAPTOMETHYL-2-(OCTYLAMINO)-1,3-PROPANEDIOL, HYDROCHLORIDE/CN
E23             1      2-MERCAPTOMETHYL-3-(O-TOLYL)-4-(3H)QUINAZOLONE/CN
E24             1      2-MERCAPTOMETHYL-3-ISOPROPYLIMIDAZO(5,1-B)THIAZOLE/CN
E25             1      2-MERCAPTOMETHYL-3-MERCAPTOPROPIONIC ACID/CN

=> S E3
L1              1 2-MERCAPTOIMIDAZOLE/CN

=> DIS L1 1 RN CCN
THE ESTIMATED COST FOR THIS REQUEST IS 1.95 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2007 ACS on STN
RN   872-35-5  REGISTRY
CN   2H-Imidazole-2-thione, 1,3-dihydro-  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   2-Imidazolemercaptan (3CI);  4-Imidazoline-2-thione (7CI);
     Imidazole-2-thiol (6CI, 8CI)
OTHER NAMES:
CN   1,3-Dihydro-2H-imidazole-2-thione;  1,3-Dihydroimidazole-2-thione;
     1,3-Vinylenethiourea;  1H-Imidazole-2-thiol;  2-Mercapto-1H-imidazole;
     2-Mercaptoimidazole;  2-Thioimidazole;  2-Thioxo-2,3-
     dihydroimidazole;  NSC 112715


=> DIS L1 1 FIDE
THE ESTIMATED COST FOR THIS REQUEST IS 4.82 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2007 ACS on STN
RN   872-35-5  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   2H-Imidazole-2-thione, 1,3-dihydro-  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   2-Imidazolemercaptan (3CI)
CN   4-Imidazoline-2-thione (7CI)
CN   Imidazole-2-thiol (6CI, 8CI)
OTHER NAMES:
CN   1,3-Dihydro-2H-imidazole-2-thione
CN   1,3-Dihydroimidazole-2-thione
CN   1,3-Vinylenethiourea
CN   1H-Imidazole-2-thiol
CN   2-Mercapto-1H-imidazole
CN   2-Mercaptoimidazole
CN   2-Thioimidazole
CN   2-Thioxo-2,3-dihydroimidazole
CN   NSC 112715
DR   55107-84-1, 4708-60-5
MF   C3 H4 N2 S
CI   COM
LC   STN Files:   ANABSTR; BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT,
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CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, IFICDB, IFIPAT, IFIUDB, MEDLINE, PIRA, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

DT.CA CAplus document type: Conference; Journal; Patent

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

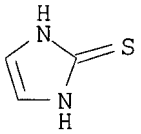
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3N2	NCNC2	5	C3N2	16.195.24	1

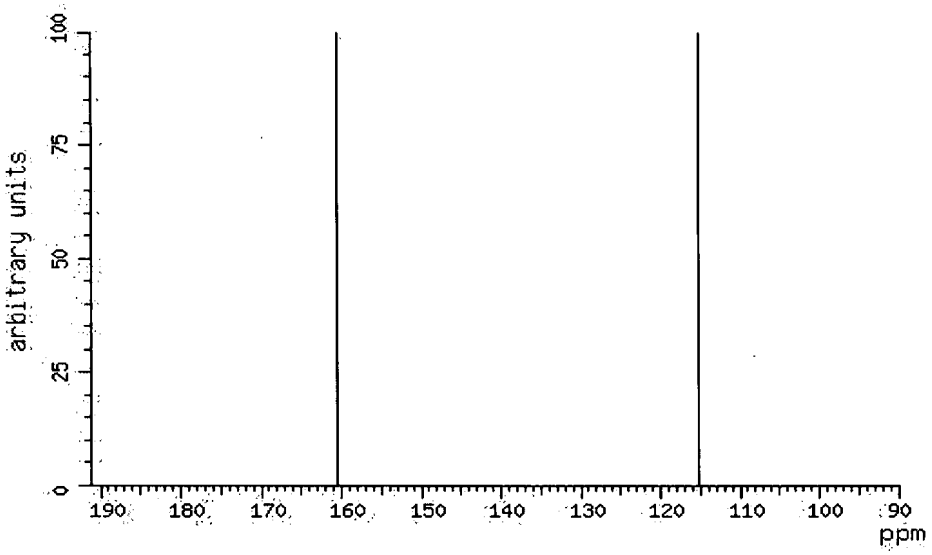


Experimental Properties (EPROP)

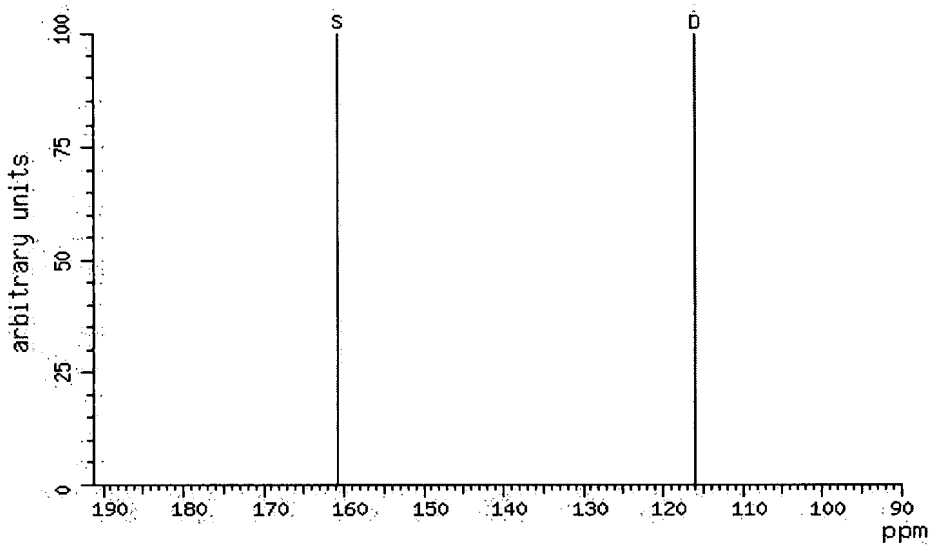
PROPERTY (CODE)	VALUE	CONDITION	NOTE
Carbon-13 NMR Spectra	Spectrum		(1) WSS
Melting Point (MP)	228-231 deg C		(2) CAS
Melting Point (MP)	225-227 deg C		(3) CAS
Melting Point (MP)	225 deg C	Solv: ethyl ether (60-29-7), acetone (67-64-1)	(4) IC

(1) Bojarska-Olejnik, Elzbieta; Bulletin of the Polish Academy of Sciences, Chemistry 1986 V34(7-8) P295-303 CAPLUS
(2) Huang, Ling; Journal of Physical Chemistry B 2006 V110(42) P20756-20758 CAPLUS
(3) Akabori, Shiro; Nippon Kagaku Kaishi (1921-47) 1931 V52, P844-50 CAPLUS
(4) Kister, Jacky; Canadian Journal of Chemistry 1979 V57(7) P813-21 CAPLUS

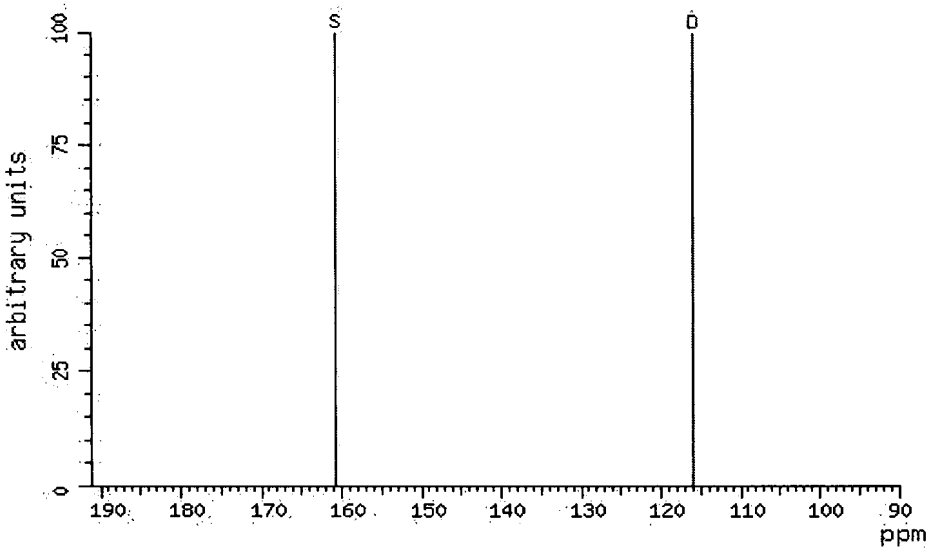
Carbon-13 NMR Spectra



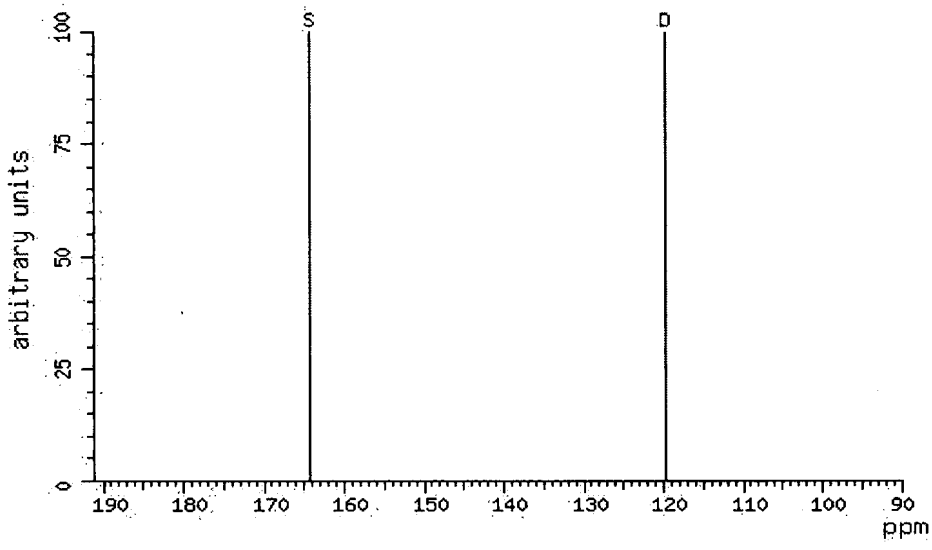
Spectrum ID: CC-03-C_SPC-9573
Temperature: 25 deg C
Solvent: dimethyl sulfoxide (67-68-5)
Spectrometer: Bruker WH-90
Source: Spectral data were obtained from Wiley Subscription Services, Inc. (US)



Spectrum ID: CNCC-63899-169S
Temperature: 28 deg C
Solvent: dimethyl sulfoxide-d6 (2206-27-1)
Standard: dimethyl sulfoxide-d6
Spectrometer: Varian CFT-20
Source: Spectral data were obtained from Wiley Subscription Services, Inc. (US)



Spectrum ID: CNUC00044836
Solvent: dimethyl sulfoxide (67-68-5)
Source: Spectral data were obtained from Wiley Subscription Services, Inc. (US)



Spectrum ID: CNCC-21269-098P
Solvent: dimethyl sulfoxide-d6 (2206-27-1)
Standard: dimethyl sulfoxide-d6
Spectrometer: Bruker WM-250
Source: Spectral data were obtained from Wiley Subscription Services, Inc. (US)

Experimental Property Tags (ETAG)

PROPERTY	NOTE
Carbon-13 NMR Spectra	(1) CAS

IR Absorption Spectra	(2) IC
Pore Size	(1) CAS
Porosity	(1) CAS
Proton NMR Spectra	(1) CAS
1 more tag shown in the MAX or ETAGFULL formats	
Silicon-29 NMR Spectra	(1) CAS
Specific Surface Area	(1) CAS
Thermal Analysis	(1) CAS
UV and Visible Absorption Spectra	(2) IC

(1) Marino, Glimaldo; Materials Science Forum 2004 V455-456, P388-392 CAPLUS

(2) Kister, Jacky; Canadian Journal of Chemistry 1979 V57(7) P813-21 CAPLUS

Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 10 25 deg C	(1)
Boiling Point (BP)	152.4+/-23.0 deg C	760 Torr	(1)
Density (DEN)	1.36+/-0.1 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	38.92+/-3.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	46.0+/-22.6 deg C		(1)
Freely Rotatable Bonds (FRB)	0		(1)
H acceptors (HAC)	2		(1)
H donors (HD)	2		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	4		(1)
Koc (KOC)	31.05	pH 1 25 deg C	(1)
Koc (KOC)	31.12	pH 2 25 deg C	(1)
Koc (KOC)	31.12	pH 3 25 deg C	(1)
Koc (KOC)	31.12	pH 4 25 deg C	(1)
Koc (KOC)	31.12	pH 5 25 deg C	(1)
Koc (KOC)	31.12	pH 6 25 deg C	(1)
Koc (KOC)	31.12	pH 7 25 deg C	(1)
Koc (KOC)	31.12	pH 8 25 deg C	(1)
Koc (KOC)	31.06	pH 9 25 deg C	(1)
Koc (KOC)	30.52	pH 10 25 deg C	(1)
LOGD (LOGD)	0.21	pH 1 25 deg C	(1)
LOGD (LOGD)	0.21	pH 2 25 deg C	(1)
LOGD (LOGD)	0.21	pH 3 25 deg C	(1)
LOGD (LOGD)	0.21	pH 4 25 deg C	(1)
LOGD (LOGD)	0.21	pH 5 25 deg C	(1)
LOGD (LOGD)	0.21	pH 6 25 deg C	(1)
LOGD (LOGD)	0.21	pH 7 25 deg C	(1)
LOGD (LOGD)	0.21	pH 8 25 deg C	(1)
LOGD (LOGD)	0.21	pH 9 25 deg C	(1)
LOGD (LOGD)	0.21	pH 10 25 deg C	(1)
LOGP (LOGP)	0.214+/-0.615	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	25 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	25 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	25 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	25 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	25 g/L	pH 4 25 deg C	(1)

Mass Solubility (SLB.MASS)	25 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	25 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	25 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	25 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	25 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	25 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	25 g/L	Unbuffered Water pH 6.15 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.25 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.25 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.25 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.25 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.25 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.25 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.25 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.25 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.25 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.25 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.25 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.25 mol/L	Unbuffered Water pH 6.15 25 deg C	(1)
Molar Volume (MVOL)	73.3+/-5.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	100.14		(1)
PKA (PKA)	11.40+/-0.30	Most Acidic 25 deg C	(1)
PKA (PKA)	-1.60+/-0.50	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	56.15 A**2		(1)
Vapor Pressure (VP)	3.50E+00 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2007 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

611 REFERENCES IN FILE CA (1907 TO DATE)
28 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
611 REFERENCES IN FILE CAPLUS (1907 TO DATE)
25 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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FULL ESTIMATED COST	14.42	14.63

STN INTERNATIONAL LOGOFF AT 08:36:14 ON 07 AUG 2007